NUMERICAL SIMULATION OF THE GAS IMMERSION LASER DOPING PROCESS IN SILICON

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Abstract

Calculations of the dopant diffusion into molten silicon during exposure to a pulsed XeCl excimer laser has been carried out. Thus, the dopant concentration profiles resulting from the Gas Immersion Laser Doping (GILD) process have been predicted. Dopant atoms may be incorporated either through a layer adsorbed on the solid silicon surface before melt, or through a uniform flux of molecules impinging on the liquid surface. These two possible physical mechanisms will be discussed.

OUTLINE

Recently a XeCl excimer laser has been used to fabricate very shallow ultra-high concentration doping profiles for VLSI devices [1]-[3]. This process relies on a dopant species being incorporated into a very shallow region of the silicon surface when it is melted by a 308nm *UV* pulsed XeCl excimer laser. The laser used in this work has an asymmetrical gaussian pulse shape with ~35 nsec FWHM, and an energy range up to 200 mJ. The doping sources that have been used are AsH_3 and B_2H_6 for n^+/p and p^+/n junctions, respectively.

With this choice of wavelenght the dissociation of the doping sources is known to be activated by pyrolysis because the gas is transparent to the laser beam. Therefore, it occurs directly on the surface of the semiconductor. The incorporation of the dopant occurs via diffusion in the liquid phase and subsequent recrystallization by liquid phase epitaxy (LPE), since the diffusion in the solid phase is negligible for the time scales involved. The energy threshold for melting (~0.7 J cm^{-2}) and the maximum melting depth for several energies have been predicted by solving the heat diffusion equation [4].

The diffusion equation for the impurities in molten silicon, including segregation effects at the advancing interface during LPE, has also been solved by means of a quasi-stationary finite differences algorithm in order to simulate the doping concentration profile resulting from one or more laser pulses. The diffusion coefficient in liquid silicon is of the order of 10^{-4} cm^2-sec^{-1} for the most common dopants (P,As,B) [5], while the segregation coefficient is ~0.3 for P and As, and ~0.8 for B in equilibrium conditions [6], but it has been reported [7] to be close to 1 during the LPE high recrystallization velocities (~3 m/s) occurring for our process. The physical mechanism of doping is contained in the boundary condition at the surface. Two models, the adsorbtion and the impingement, outlined in Fig.1, will now be discussed.

The incorporation of the dopant into the liquid silicon may begin from a molecular layer adsorbed on the solid surface before the melting threshold has been reached. Several experiments have been carried out in order to estimate this layer. In an AsH_3 environment we have measured an adsorbed layer of $N=1x10^{14}$ atoms cm^{-2} for each pulse which corresponds to about 10% of a monolayer. The boundary condition for the diffusion equation is a layer of N molecules on the surface at the time the melt begins, whose thickness is given by the step (~10 A) used for the numerical computation. An attempt is being made to understand how

this layer depends on the operative conditions (pressure, etc.), and whether the adsorbtion saturates or more monolayers may be added.

The second factor, which may also play a role giving an additional contribution to the doping, is the impingement of the thermally vibrating molecules of the gas on the liquid surface. This has been modeled by entering a constant flux over the time during which the surface remains molten. This flux is related to a sticking coefficient, which is the fraction of molecules striking the surface solubilized in the liquid phase. This contribution can be experimentally estimated by changing the pressure or the melt duration (i.e. the pulse energy). A sticking coefficient < 0.1 is compatible with our experimental results. With today's requirements for shallow junctions near-thresold laser energies are needed and the adsorbtion effect becomes more prevalent.

References

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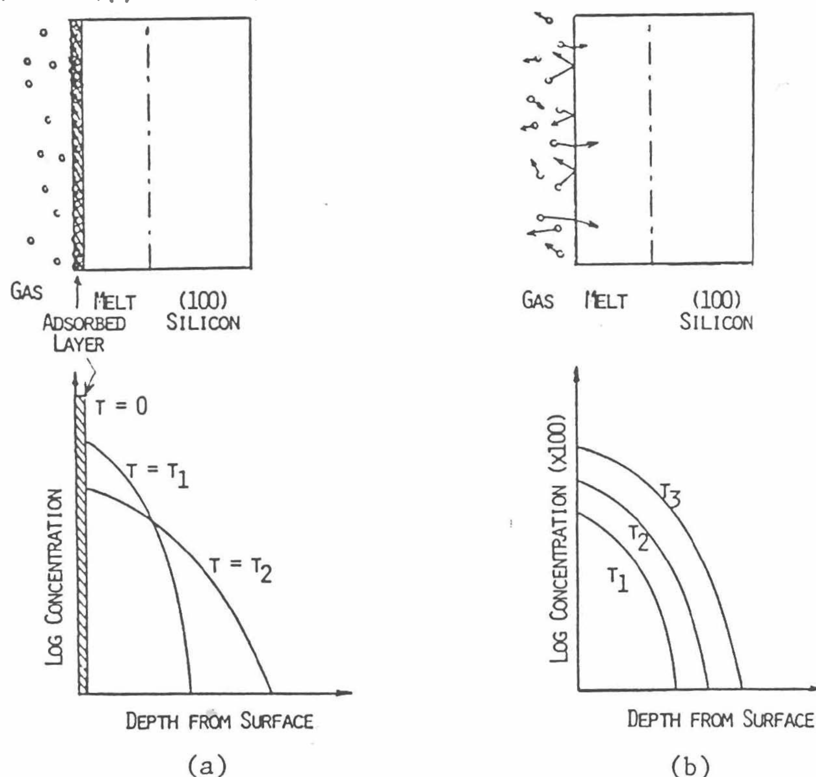

Fig. 1. Schematic of the adsorbtion (a) and the impingement (b) models of GILD in silicon.